

Equation of state of compressed matter: A simple statistical model.

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Abstract

We propose a simple approach for studying systems of compressed matter based on the Thomas-Fermi statistical model of single atom. The central point of our work is the development of the concept of “statistical ionization” by compression; in simple terms, we calculate the fraction of electrons within the atom whose positive energy, due to the compression, exceeds the negative binding energy electron-nucleus. Next we extend this concept from a single atom to macroscopic systems and write the corresponding equation of state. Positive aspects as well as limitations of the model are illustrated and discussed through all the paper.

Author Keywords: Thomas-Fermi, compressed atoms, statistical ionization, equation of state.

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A. Introduction

The Thomas-Fermi model (see the original work of Fermi [1], or any textbook of condensed matter, e.g. [2]) represents a simple and powerful tool for the basic investigation of atomic properties. Although the theoretical framework is highly simplified, quantitative as well as qualitative results are surprisingly good; for example, in the description of compressed atoms, theoretical [3] as well as experimental [4] work testify the validity of such an approach. In the following part of this work we focus the attention on this particular case (atoms under pressure) and develop the concept of “statistical ionization” by compression; we define the total energy, calculated in a classical way, of the compressed atom as a function of the distance from the point-like nucleus and using the corresponding solution of the Thomas-Fermi equation we are able to define the region within the atom characterized by positive energy, as a consequence we can estimate the average number of electrons (fraction of electrons) whose antibinding energy (again in a classical sense) is dominant with respect to the binding energy electron-nucleus; the term “average” must be interpreted in the sense that we do not refer to the electrons as single particles characterized by specific quantum numbers, but we refer to them as the results of the process of integration of an average distribution of charge (i.e. the electron density) over a certain region of the real space. Of course, it must be clear, that we do not intend to refer to a such ionization mechanism as a realistic one since the electron ionization does not depend on the distance from the nucleus and involves more complicated quantum effects which cannot be considered by this model; what we intend to do is simply to estimate in a classical statistical way the effects of the compression on the kinetic energy, electron-electron and electron-nucleus interaction. Finally from the single atom, we extend the model to condensed matter systems introducing, with a statistical approach, the atomistic model into a multiatomic system. The paper is organized as follows: after a basic review of the Thomas-Fermi model necessary for the next part of the paper, we describe the process of “statistical ionization” by compression, finally the equation of state of compressed matter is derived accordingly to the model illustrated

in the previous section.

I. THE THOMAS-FERMI MODEL

In this section we will follow the procedure to obtain the Thomas-Fermi equation reported in reference [2]. The Fermi statistics at zero Kelvin is applied to study the bound state of an atom characterized by a statistical number of electrons. The N electrons of the system are treated as a degenerate Fermi gas confined in a region of the real space by a spherical potential $V(r)$ which goes to zero in the limit of $r \rightarrow \infty$; it is supposed that the potential is slowly varying for distances which are large compared to the De Broglie wavelength, so that in the volume where $V(r)$ is approximatively constant we can think that there are enough electrons to justify the statistical approach of the electrons as a Fermi gas; moreover the large number of particles allow one to think that most of them have got an high principal quantum number in order to justify the application of semiclassical methods. The aim of the Thomas-Fermi model is to calculate $V(r)$ and the electron density $\rho(r)$; to do so, these two quantities are related to each other in the following way. The total energy of an electron can be written as:

$$p^2/2m + V(r) \tag{1.1}$$

with m the mass of an electron, since the maximum value of the kinetic energy an electron can reach is the Fermi energy, the most energetic electrons of the system will be characterized by a total energy:

$$E_{max} = E_{Fermi} + V(r). \tag{1.2}$$

It is clear that E_{max} does not depend on r because if not all the electrons would migrate in the region in correspondence of which such a quantity has a minimum. The Fermi momentum depends on r since $p_{Fermi}^2/2m = E_{max} - V(r)$, and that it can also be expressed as:

$$p_{Fermi} = \hbar(3\pi^2)^{1/3}(\rho(r))^{1/3} \tag{1.3}$$

where $\rho(r) = N/V$, N total number of electron, V the volume where they are confined (see for example [5]); the combination of these two relations leads to :

$$\rho(r) = \frac{(2m/\hbar^2)^{3/2}}{3\pi^2} [E_{max} - V(r)]^{3/2} \quad (1.4)$$

in the region classically forbidden where $E_{max} - V(r) < 0$ we impose $\rho(r) = 0$. Next the electrostatic potential is defined as:

$$\psi(r) = -\frac{V(r)}{e} \quad (1.5)$$

with $\psi_0 = -E_{max}/e$ positive constant being e the electron charge. Defining:

$$\phi(r) = \psi(r) - \psi_0 \quad (1.6)$$

it follows that $\rho(r)$ and $\phi(r)$ are related as:

$$\rho(r) = \frac{(2m/\hbar^2)^{3/2}}{3\pi^2} [e\phi(r)]^{3/2} \quad (1.7)$$

for $\phi(r) \geq 0$ and $\rho(r) = 0$ for $\phi(r) \leq 0$. Implementing the relations above into the Poisson equation we obtain:

$$\frac{1}{r} \frac{d^2}{dr^2} [r\phi(r)] = \frac{e(2m/\hbar^2)^{3/2}}{3\pi^2 \epsilon_0} [e\phi(r)]^{3/2} \quad (1.8)$$

for $\phi(r) \geq 0$

and

$$\frac{1}{r} \frac{d^2}{dr^2} [r\phi(r)] = 0 \quad (1.9)$$

for $\phi(r) \leq 0$ being ϵ_0 the dielectric constant. For $r \rightarrow 0$ the predominant term of the electrostatic potential is due to the nucleus, it follows that:

$$\lim_{r \rightarrow 0} r\phi(r) = \frac{Ze}{4\pi\epsilon_0} \quad (1.10)$$

where Ze is the charge of the nucleus; in addition to the above condition we have to add the normalization condition $4\pi \int_0^{r_0} \rho(r) r^2 dr = N$, where r_0 is the radius of the atom. At this point we introduce the dimensionless variable and function:

$$r = bx \quad (1.11)$$

$$r\phi(r) = \frac{Ze}{4\pi\epsilon_0}\chi(x) \quad (1.12)$$

where $b = \frac{3\pi^2}{2^{7/3}}a_0Z^{-1/3}$ with a_0 is the Bohr radius. The definitions reported above imply the following relation:

$$\rho(r) = \frac{Z}{4\pi b^3}(\chi(x)/x)^{3/2} \quad (1.13)$$

for $\chi(x) \geq 0$ and $\rho(r) = 0$ for $\chi(x) < 0$. Finally the dimensionless equation 1.8 can be written in the form known as the Thomas-Fermi equation:

$$\frac{d^2}{dx^2}\chi(x) = x^{-1/2}\chi(x)^{3/2} \quad (1.14)$$

for $\chi(x) \geq 0$

and

$$\frac{d^2}{dx^2}\chi(x) = 0 \quad (1.15)$$

for $\chi(x) < 0$;

the condition in $x = 0$ becomes $\chi(0) = 1$. It is important to notice that equation 1.14 is independent from the atomic species, in other words is universal and the nature of the atom can be reintroduced in the scaling factor; this fact will play an important role in the development of our model.

A. Solutions of the Thomas-Fermi equation

Since equation 1.14 is a second order differential equation and the boundary condition in $x = 0$ specifies only one of the two required conditions to have a unique solution, it will exist a class of solutions $\chi(x)$ which satisfies the condition in $x = 0$ and for a specific solution will depend on the value $\chi'(x)_{x=0}$ (the symbol ' means derivative with respect to x). The general solution of the Thomas-Fermi equation can be classified in three categories:

- (1) Asymptotic solution obtained for $\chi'(x)_{x=0} \approx -1.576...$
- (2) Solution which goes to zero for finite values of x , i.e $x = x_0$, for $\chi'(x)_{x=0} < -1.576...$
- (3) Solution which diverges for large x , for $\chi'(x)_{x=0} > -1.576...$

We do not report a pictorial description of these solutions, since it can be found in details in reference [2]. The physical meaning of the three categories of solutions can be understood examining the normalization condition. In fact:

$$N = Z \int_0^{x_0} x^{1/2} \chi(x)^{3/2} dx \quad (1.16)$$

leads to

$$N = Z[x\chi'(x) - \chi(x)]_0^{x_0} \quad (1.17)$$

and finally to :

$$\frac{N - Z}{Z} = x_0 \chi'(x_0) - \chi(x_0). \quad (1.18)$$

In the asymptotic case we have that $\chi'(x)$ goes to zero as $\chi(x)$ for large x so we have the neutral atom with the infinite radius; in the second case we have that $\chi(x_0) = 0$ but $\chi'(x_0)x_0 \neq 0$ so we obtain $N - Z < 0$ being $\chi'(x_0) < 0$, i.e positive ions; in the third case which is the one particularly relevant for our work, we have:

$$\chi'(x_0)x_0 - \chi(x_0) = 0 \quad (1.19)$$

where x_0 is smaller than the radius of the neutral atom (infinite as stated before) so that such a solution is interpreted as the solution describing compressed neutral atoms.

II. STATISTICAL IONIZATION BY COMPRESSION

In this section we will illustrate the concept of statistical ionization by compression in physical as well as mathematical terms. First, we make the ideal picture of the atom as composed of concentric shells of infinitesimal thickness around the point-like nucleus, in this approach the total energy within the atom at a certain distance from the nucleus is

represented by the sum of the energy of each single infinitesimal shell contained in the volume corresponding to that distance, or equivalently, for a continuum of shells, by the integral over that volume. Next, we write the total energy of the atom in terms of solutions of the Thomas-Fermi equation for compressed atoms within the idealized shells' approach; this simply leads to a semianalytical function of the distance from the nucleus. At this point it can be noticed that the distance from the nucleus at which this function has got a minimum corresponds to the shell characterized by a null contribution to the total energy; from a physical point of view this means that this shell is characterized by the exact balance between binding and antibinding energy or in other words is the distance at which the attractive potential between the nucleus and the electrons starts to be less dominant than the electron-electron and kinetic contributions. Once this distance has been found, it is automatically defined a region within the atom, characterized by a positive energy; integrating over this region, one obtains the average number of electrons whose binding interaction with the nucleus can be considered negligible, i.e. they can be, with a good approximation, considered free. As stated before, this process is not meant to reproduce a realistic ionization, but it represents a simple mechanism which in terms of classical interactions between the physical elements of the system helps one to picture out the balancing process between the reduced volume available to the atom and the topological readjustment of the electron density; the average number of electrons considered free must be interpreted as a fraction of electrons which can be represented as a non interacting electron gas. It must be underlined that this is not obvious, since the Thomas-Fermi model is based on the hypothesis of non interacting electron gas and we use this description to define an electron-electron interaction and calculate the fraction of electrons free from the nucleus; the argument which one can use to solve this critical point is that once the electron distribution is defined via the Thomas-Fermi equation as a further step the electrostatic interaction between electrons can be calculated as a usual classical self-interacting charged sphere and that the initial hypothesis of non interacting electrons is just a simplification to obtain at a first step a reasonable atomistic electron distribution; at the same time the "ionized"

electrons can be interpreted as non interacting fermionic electron gas in a less approximate way than the total number of electrons considered initially in the Thomas-Fermi model since these former do not feel the nucleus attraction. It must be clear , as stated also before, that a realistic process of ionization cannot depend on the distance of the electrons from the nucleus, in our model this simply represents a sort of classical way to describe the process and is related to the semiclassical and statistical nature of the Thomas-Fermi model; this means that it makes sense within a semiclassical framework but not for example in a proper quantum treatment.

A. The Total Energy Function or Ionization Function

In this section we write the total energy of the atom as a distance from the nucleus using the solutions for the compressed atoms. In a classical approach, the total energy of the electrons “located” at distance R from the nucleus is (see also reference [6]):

$$E(R)_{total} = E(R)_{kinetic} + E(R)_{electron-electron} + E(R)_{electron-nucleus} \quad (2.1)$$

1. The Kinetic Energy

The kinetic energy is the energy of a fermionic gas in a sphere at zero Kelvin:

$$E(R)_{kinetic} = \int_0^R 4\pi r^2 \int_0^{p_{Fermi}(r)} \frac{4\pi p^4}{m\hbar^3} dp \quad (2.2)$$

this can be written in terms of Thomas-Fermi adimensional quantities as:

$$E_{kinetic}(s) = \frac{3Z^2 e^2}{5b} \int_0^s \chi(x)^{5/2} x^{-1/2} dx \quad (2.3)$$

where $s = R/b$ and $x = r/b$ being b the same as defined before. This integral can be simplified in a useful semianalytical form (what we mean is that the final form is analytical in χ and χ' , but is globally semianalytical since χ and χ' are numerical solutions, as functions of the

dimensionless distance from the nucleus). Considering that $\chi''(x) = \chi^{3/2}(x)/x^{1/2}$, where χ'' is the second derivative with respect to x , the integral can be rewritten as:

$$\int_0^s \chi(x)^{5/2} x^{-1/2} dx = \int_0^s \chi'' d\chi \quad (2.4)$$

which is equivalent to:

$$\int_0^s \chi'' d\chi = \int_0^s \chi d\chi' \quad (2.5)$$

taking into account that $\chi(0) = 1$ and integrating by parts, we obtain:

$$\int_0^s \chi d\chi' = [\chi(x)\chi'(x)]_0^s - \int_0^s \chi' d\chi. \quad (2.6)$$

The the second term of the right side of the previous equation can be expressed as:

$$- \int_0^s \chi' d\chi = - \int_0^s (\chi')^2 dx \quad (2.7)$$

which, using again the integration by parts and the properties of the Thomas-Fermi equation, becomes:

$$- \int_0^s (\chi')^2 dx = [-(\chi(x)')^2 x]_0^s + \left[\frac{4}{5} \chi(x)^{5/2} x^{1/2} \right]_0^s - \frac{2}{5} \int_0^s \chi(x)^{5/2} x^{-1/2} dx. \quad (2.8)$$

It follows that:

$$\int_0^s \chi(x)^{5/2} x^{-1/2} dx = [\chi(x)\chi'(x)]_0^s - [(\chi(x)')^2 x]_0^s + \left[\frac{4}{5} \chi(x)^{5/2} x^{1/2} \right]_0^s - \frac{2}{5} \int_0^s \chi(x)^{5/2} x^{-1/2} dx. \quad (2.9)$$

Finally:

$$E(s)_{kinetic} = \frac{3Z^2 e^2}{7b} \left[\chi(s)\chi'(s) - \chi'(0) - (\chi'(s))^2 s + \frac{4}{5} (\chi(s))^{5/2} s^{1/2} \right]. \quad (2.10)$$

2. The Electron-Nucleus Interaction

In this part, we write the electron-nucleus interaction in terms of the Thomas-Fermi quantities. The electron-nucleus interaction is written as:

$$E_{e-n}(R) = -Ze^2 \int_0^R 4\pi r^2 \frac{\rho(r)}{r} dr \quad (2.11)$$

and within the Thomas-Fermi approach becomes:

$$E_{e-n}(s) = -\frac{Ze^2}{b} \int_0^s [\chi(x)]^{3/2} x^{-1/2} dx = -\frac{Ze^2}{b} \int_0^s \chi(x)'' dx. \quad (2.12)$$

Finally, integrating by parts we obtain:

$$E_{e-n}(s) = \frac{Ze^2}{b} [\chi'(s) - \chi'(0)]. \quad (2.13)$$

3. The Electron-Electron Interaction

In the same fashion of the previous calculations, we repeat the procedure for the electron-electron interaction.

$$E_{e-e}(\mathbf{R}) = \frac{e^2}{2} \int_V \rho(\mathbf{r}) d\mathbf{r} \int_{V_0} \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' \quad (2.14)$$

the bold letters indicate that the related quantity is in Cartesian coordinates, V is a varying spherical region within the atom while V_0 is the total volume of the atom. This integral can be simplified in terms of Thomas-Fermi quantities in the following way (see also reference [6]):

$$E_{e-e}(\mathbf{s}) = \frac{1}{2} \frac{Z^2 e^2}{b} \int_0^s [\chi(x)]^{3/2} x^{1/2} dx \left[\frac{1}{x} \int_0^x [\chi(x')]^{3/2} (x')^{1/2} + \int_0^{s_0} [\chi(x')]^{3/2} (x')^{1/2} \right] \quad (2.15)$$

where $s_0 = R_0/b$, being R_0 the total radius of the atom. Applying the Thomas-Fermi equation $\chi'' = \chi^{3/2}/x^{1/2}$, and integrating by parts we obtain:

$$E_{e-e}(\mathbf{s}) = \frac{1}{2} \frac{Z^2 e^2}{b} \int_0^s [\chi(x)]^{3/2} x^{1/2} dx [-\chi(x)/x + \chi(0)/x + \chi'(x_0)] \quad (2.16)$$

and this gives:

$$\int_0^s [\chi(x)]^{5/2} x^{-1/2} dx + \chi(0) \int_0^s [\chi(x)]^{3/2} x^{-1/2} dx + \chi'(x_0) \int_0^s [\chi(x)]^{3/2} x^{1/2} dx \quad (2.17)$$

the first term is equivalent to the integral of the kinetic energy, the second is equivalent to the integral of the electron-nucleus energy multiplied by 2, the integral of the third term

can be solved in the same way as the two inner integrals of the electron-electron energy in equation 2.16; it follows that the final form for the electron-electron energy in units of $Z^2 e^2 / b$ is:

$$\begin{aligned}
E_{e-e}(s) = & \frac{1}{14}\chi(s)\chi'(s) + \\
& \frac{3}{7}\chi'(0) - \frac{1}{14}s(\chi'(s))^2 + \\
& \frac{2}{35}s^{1/2}\chi(s)^{5/2} - \frac{1}{2}\chi'(s) + \frac{1}{2}s\chi'(s_0)\chi'(s) - \frac{1}{2}\chi'(s_0)\chi(s)
\end{aligned} \tag{2.18}$$

4. Final Form of the Ionization Function and Qualitative Numerical Results

In this part we give the final form of the total energy, and show a pictorial representation of its curve for three different degrees of compression. Combining the results of the integration performed in the previous sections we can write the total energy (in arbitrary units) as:

$$\begin{aligned}
E_{tot}(x) = & \frac{1}{2}\chi(x)\chi'(x) - \frac{1}{2}[\chi'(x)]^2x + \chi'(0) + \frac{14}{35}[\chi(x)]^{5/2}x^{1/2} \\
& - \frac{3}{2}\chi'(x) + \frac{1}{2}x\chi'(x_0)\chi'(x) - \frac{1}{2}\chi'(x_0)\chi(x)
\end{aligned} \tag{2.19}$$

where we formally replaced s with x , previously used as the integration variable. The average number of “ionized” electron is given by:

$$N_i = Z \int_{x_i}^{x_0} x^{1/2}[\chi(x)]^{3/2}dx = Z[\chi(x_i) - x_i\chi'(x_i)] \tag{2.20}$$

x_i is the dimensionless distance at which the minimum of the ionization function is located. We studied numerically the behavior of the ionization function for three different degrees of compression, which in mathematical terms means that we used three different solutions of the Thomas-Fermi equation corresponding to three different initial conditions on $\chi'(0)$; figure 1, shows the qualitative behavior of such a function; indeed a minimum is found, and the corresponding dimensionless distance can be used for calculating the average number of “ionized” electrons. As we expect for very compressed atoms ($\chi'(0)$ less negative) the distance at which the positive contributions to the energy start to be dominant (with respect

to the less compressed atoms) is shorter, or in simple terms, the average number of “ionized” electrons is larger. This of course simply shows that the model does not present an unphysical behavior and is qualitatively reasonable but, as stated before, it should not be directly compared with specific ionization studies.

III. EQUATION OF STATE OF SYSTEMS UNDER PRESSURE

In this part we will apply the model developed before to write the equation of state of systems under pressure. The original work of the ionization by compression [7] was developed for describing astrophysical systems at high density and consequently at extreme pressure (white dwarfs). In this case the usual basic approach used in literature (see for example [5]) consists in considering the atoms fully ionized and the equation of state is written in the approximation of the electrons a perfect Fermi gas in the ground state, while the nuclei are not suppose to contribute to the pressure. In our case the approximation is less crude since we do estimate the average number of electrons per atom which at a given pressure or equivalently at a given density of matter of the system (in terms of the inverse of the volume of the atom) can be considered free from the nucleus attraction so that for them it is more appropriate to apply the properties of the perfect Fermi gas. In a large system of a single species of atoms we can imagine the compressed atom as the one described by the Thomas-Fermi model and the pressure experienced by the atom is the same the itself atom produces on the system in a situation of equilibrium. It follows that if we consider all the electrons of the atom as a Fermi gas, the equation of state is:

$$P = 3\pi^{4/3} \frac{\hbar^2}{5m_e} \left[\frac{N}{V} \right]^{5/3} \quad (3.1)$$

where N is the total number of electrons of the atom and V the corresponding volume; this formula is not fully justified when we use our approach of partial ionization since in this case the equation takes the form:

$$P = 3\pi^{4/3} \frac{\hbar^2}{5m_e} \left[\frac{N_i(V)}{V} \right]^{5/3} . \quad (3.2)$$

where $N_i(V)$ is the average number of “ionized” electrons. The approximation of considering the “ionized” electrons as a Fermi gas, should be introduced in the equation of state in a statistical way, since the pressure is a statistical quantity and must be calculated using a statistically number of electrons; the number of “ionized” electrons for single atom is clearly not fulfilling such a requirement. To do so, we use the following procedure, we take a volume inside the many-atom system containing a large number of atoms N_a which we consider under the same physical conditions. It follows that the equation of state can be written as:

$$P = 3\pi^{4/3} \frac{\hbar^2}{5m_e} \left[\frac{N_a N_i(V)}{N_a V} \right]^{5/3} \quad (3.3)$$

in this case the total number of free electrons contributing to the pressure is $N_a N_i(V)$ and the total volume in which they are confined is $N_a V$; the above equation obviously reduces to equation 3.2. In simple terms, the “ionized” electrons are considered a Fermi gas in the ground state while the remaining electrons are approximate as a frozen core containing also the nucleus, in the same fashion, with due differences, of the pseudopotential approach used in modern first principles calculations of condensed systems. The equation obtained can be extended to any system, regardless of the size; of course we expect that large systems at relatively high pressure represent better the statistical framework required by the approximations done, this is the reason we developed the procedure keeping in mind the case of astrophysical objects.

IV. DISCUSSION AND CONCLUSIONS

As stated all over the paper, this is a very simple model, we do not expect to obtain valid precise quantitative results; however when used in a semiclassical statistical framework, it could give valid indications. Certainly the approach described in reference [5] for large systems under pressure represents a crude approximation; the same can be said for our model, but once the approximation of “frozen core” electrons is accepted, the “ionized”

electrons well represent an ideal Fermi gas. Of course when the pressure becomes extremely high, relativistic effects as well as nuclear processes (e.g. inverse β -decay) become relevant and the approximation of non-relativistic Fermi gas is not justified anymore; this means that our model is valid up to a certain degree of compression. Moreover, the model can be applied in principle to any species of atoms by simply scaling all the quantities by the factor Z , this is a relevant property which makes the ionization function universal. However when more sophisticated models of the Thomas-Fermi equation are used the universality of the description is lost (for example when electronic exchange and correlation effects are included [3]). We expect the model to be less valid for ordinary condensed systems under pressure where do not exist fully idealized statistical conditions and the details of a quantum description become relevant. Nevertheless also in this case our approach can be useful to have a first estimate of the compression process; in particular in many self consistent first principles calculations where the pseudopotential approach is used, our model could be used to estimate the number of “ionized” electrons so that at the first step of the self-consistency they can be represented by a plane-wave electron wavefunction while the remaining electrons can be approximate by a frozen core or by closed shell orbitals centered on the nucleus; this could speed up the convergence of the self-consistent process. In conclusion, we think that due to the its simplicity and feasibility, our model, when is used in a proper context, represents a useful tool for the basic investigation of statistical properties of compressed systems.

V. LATER CORRECTION:PHYSICA A295 562 (2001)

Eq. (3.4) right hand side should be

$$\int_0^s \chi'' \chi dx \text{ instead of } \int_0^s \chi'' d\chi.$$

The third integral on the right hand side of Eq.(3.15) should be

$$\int_x^{s_0} [\chi(x')]^{3/2} (x')^{-1/2} \text{ instead of } \int_x^{s_0} [\chi(x')]^{3/2} (x')^{1/2}.$$

Eq. (3.17), the sign of the first integral is $-$.

Eq. (3.18), for the first and third term on the right hand side is $-5/14$ instead of $1/14$ the multiplicative factor, for the fourth term is $-10/35$ instead of $2/35$, and the fifth term is minus instead of $+$.

Eq. (3.19), for the first and second term on the right hand side is $1/14$ instead of $1/2$ the multiplicative factor, for the fourth term is $2/35$ instead of $14/35$, and for the fifth term is $-1/2$ instead of $-3/2$. The rest remains unaltered.

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REFERENCES

- [1] E.Fermi, Rend.Accad.Naz.Lincei, **6** (1927) 602..
- [2] B.H.Bransden,C.J.Joachian, *Physics of Atoms and Molecules* (Longman Scientific and Technical, New York)
- [3] R.P.Feynmann, N.Metropolis, E.Teller, *Phys.Rev.* **75** (1949) 1561.
- [4] R.F.Trunin, M.A.Podurets, G.V.Simakov, L.V.Popov, B.N.Moiseev, *Sov.Phys.JETP* **35** (1972) 550.
- [5] L.Landau, M. J. Kearsley , E.M.Lifshits, *Statistical Physics: Part 1* (Butterworth-Heinemann, Oxford, 1980).
For this work the italian version was used:
L.Landau, E.M.Lifshits, L.P.Pitaevskij, *Fisica Statistica* (Editori Riuniti, Edizioni Mir 1978)
- [6] S.L.Shapiro, S.A.Teukolsky, *Black Holes, White Dwarfs and Neutron Stars* (John Wiley & Sons, 1983)
- [7] L.Delle Site, *Tesi di Laurea*, La Sapienza, first University of Rome 1995.

FIGURES

FIG. 1. The total energy of the atom (or equivalently the ionization function as we also address to it) as a function of the dimensionless distance from the nucleus for three different degrees of compression; the dimensions are arbitrary since only the qualitative behavior is relevant; both qualitative as well as quantitative behavior do not have a physical sense for a distance which is larger than the atom's radius, accordingly to the interpretation of the solutions of the Thomas-Fermi equation for compressed atoms.

